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Development of a MELCOR Sodium Chemistry (NAC) Package – FY17 Progress

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Abstract

This report describes the status of the development of MELCOR Sodium Chemistry (NAC) package. This development is based on the CONTAIN-LMR sodium physics and chemistry models to be implemented in MELCOR. In the past three years, the sodium equation of state as a working fluid from the nuclear fusion safety research and from the SIMMER code has been implemented into MELCOR. The chemistry models from the CONTAIN-LMR code, such as the spray and pool fire models, have also been implemented into MELCOR. This report describes the implemented models and the issues encountered. Model descriptions and input descriptions are provided. Development testing of the spray and pool fire models is described, including the code-to-code comparison with CONTAIN-LMR. The report ends with an expected timeline for the remaining models to be implemented, such as the atmosphere chemistry, sodium-concrete interactions, and experimental validation tests.

ACKNOWLEDGMENTS

This work was overseen and managed by Matthew R. Denman (Sandia National Laboratories). In addition, we appreciate that Brad J. Merrill of Idaho National Laboratory (INL) provided us the modification of the MELCOR source code for the sodium work done at INL. This work is supported by the Office of Nuclear Energy of the U.S. Department of Energy work package number AT-17SN170204 and NT-18SN05030102.

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NOMENCLATURE

Abbreviation	Definition
BRISC	Burner Reactor Integrated Safety Code
CSTF	Containment Systems Test Facility
CV	Control volume
CVH	Control volume hydrodynamics
DBA	design basis accident
EOS	equations of state
FSD	Fusion Safety Database
INL	Idaho National Laboratory
LWR	Light water reactor
NAC package	Sodium chemistry package
NRC	Nuclear Regulatory Commission
SFR	sodium fast reactor
SNL	Sandia National Laboratories
SLAM	sodium limestone ablation model

1. INTRODUCTION

This report is a continuation of the previously published reports for the MELCOR/CONTAIN-LMR Integration Project [Humphries 2014, Humphries 2016, Humphries 2016a]. Unlike the previously published reports—which were cumulative reports—this report focuses on the sodium chemistry (NAC) models that either are implemented or will be implemented into MELCOR.

MELCOR [Humphries 2015] and CONTAIN [Murata 1997], which have been employed by the U.S. Nuclear Regulatory Commission (NRC) to support light water reactor (LWR) licensing, have been used for source terms, Level 2 and Level 3 probabilistic analyses, and containment design basis accident (DBA) analysis. Both codes were developed at Sandia National Laboratories (SNL) for the NRC. To prepare for future regulatory needs, new models are being added to the MELCOR code to simulate sodium fast reactors (SFRs) supported by U.S. Department of Energy. Sodium properties and equations of state (EOS), such as from the SIMMER (SAS4A) code [Cahalan 1994, Dunn 2012], have been implemented into MELCOR to replace the water properties and its EOS as reported previously [Humphries 2014a]. Additional sodium-related models to address DBA can now be implemented into MELCOR.

Figure 1-1 shows the sodium chemistry in the containment of a pool-type SFR design. As shown in this figure, much of the sodium chemistry phenomena for the containment have been modeled in CONTAIN-LMR [Murata 1993, Scholtyssek 1994]. Note that the atmospheric chemistry model developed for the CONTAIN/LMR code does not have an experimental database available for validation of that model. Alternatively, we provide a verification of the MELCOR implementation of that model by performing a code-to-code comparison with the CONTAIN2-LMR code. CONTAIN2-LMR is based on the CONTAIN2 code but with the LMR models from CONTAIN-LMR and is only used for the code-to-code comparison within SNL and will not be available for general distribution.

This report documents the developmental status of the sodium chemistry (NAC) package in MELCOR.

The overall objective of this project is to implement sodium chemistry models from CONTAIN-LMR [Murata 1993] into MELCOR. The models from CONTAIN-LMR include:

- Sodium spray fire
- Sodium pool fire
- Sodium atmospheric chemistry
- Sodium-concrete interaction (or reaction)

Even though CONTAIN-LMR did include other models, only sodium models that are important to metal fuel/pool type SFR designs are considered.

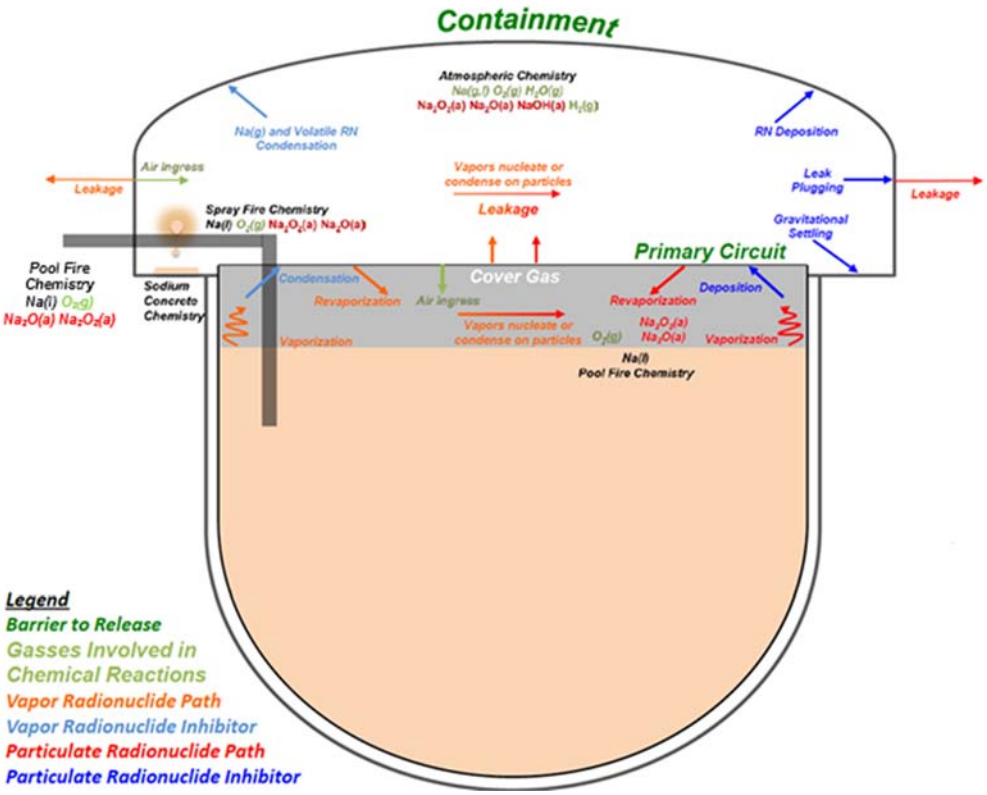


Figure 1-1. Graphical Representation of the Sodium Chemistry Models for Atmosphere, Spray, and Pool. Adopted from ANL-ART-3 [Grabaskas 2015].

In this report, we first describe the development of the NAC package into MELCOR. The NAC package is to house all sodium chemistry models associated with SFR applications. We first describe the theory and origins of the sodium models and the associated coding from the CONTAIN-LMR code be included in the NAC package in Chapter 2. Chapter 3 discusses the input descriptions, plot variables, and associated inputs. Chapter 4 describes the testing of the implemented sodium models. Conclusions are given in Chapter 5. Chapter 6 provides the timeline to complete any sodium chemistry models that are yet to be implemented into MELCOR.

2. SODIUM CHEMISTRY MODELS

This chapter describes the implementation effort of the CONTAIN-LMR sodium models to date. MELCOR currently only allows a single working fluid (i.e., condensable) in a given problem though ongoing work may permit multiple working fluids in the problem as long as they are never in the same control volume. . Note that work is being performed to allow multiple working fluids to be modeled in an input model as long as they are not defined in the same control volume (CV) or in CVs connected by flow paths. Without the ability to add water as a condensable, the only way to model both sodium and water in a given problem is to treat water as an aerosol. As an aerosol, water would have a vapor pressure associated with the transition from liquid to gas and would be available for reactions with other species but otherwise would be treated as a trace material with no heat capacity and no other hydrodynamic effect. Without the ability to add water as a condensable, the only way for us to model both sodium and water in a given problem is to treat water as an aerosol.

Further complicating the problem when implementing sodium into MELCOR is the treatment or the definition of the ambient temperature. The typical ambient temperature in the containment or experiment room is about 290 to 300 K, which is below the boiling point of water and above the water freezing point of 273 K. For sodium reactors, particularly in the containment volume, the ambient temperature in the volume may be on the order of 290 to 300 K while the freezing point of sodium is 371 K. This poses an issue with MELCOR, since MELCOR assumes that the ambient temperature is above the coolant's freezing point for the working fluid of water. To overcome this issue for SFRs (a room with the presence of water and a source of sodium) MELCOR requires the user to place an input record, called CVH_ALLOWCOOLATM to permit this situation. When sodium liquid is sourced in the problem, the atmosphere temperature needs to be above the coolant's freezing point. If not, the code will abort due to the temperature below the sodium freezing point, which aborts any extrapolation of the sodium property data. To overcome this issue and permit the extrapolation of the liquid sodium property data below sodium freezing temperature, the use of new ALLOWNATOFREEZE flag at executions should be invoked. The extension of the equations of state to permit freezing of sodium was challenging and it was important to ensure that any modifications do not compromise the existing supplication to light water reactor applications.

SAND91-1490 describes a number of containment related models for sodium (see **Table 2-1**). In terms of the model implementation as shown in, only items 1 to 3 and item 5 have and will be implemented into MELCOR.

Table 2-1. Implementation Status of the CONTAIN-LMR Sodium Models for MELCOR

No	Model	Description
1	Atmospheric Chemistry	This model allows atmospheric constituents to interact chemically to form a stable compound. The chemical reactions considered include those for sodium. The designs of the MELGEN input and data structure have been partially implemented into MELCOR. Note that water in MELCOR is treated as water aerosol. The sodium-induced hydrogen burn was not modeled.
2	Sodium Spray Fires	This model allows the treatment of the combustion of sodium spray resulting from an energetic event that causes droplets of sodium spraying out of the reactor system. The designs of the MELGEN input and data structure have been implemented. Testing and debugging is in progress.
3	Sodium Pool Fires	This pool fire model simulates the chemical reaction between sodium located in a pool and the oxygen in the atmosphere above the pool. The designs of the MELGEN input and data structure have been implemented. Testing and debugging are in progress.
4	Two-Condensable Option/Condensate Removal	This option allows the modeling of the condensation, evaporation, and boiling of both sodium and water within a single calculation. This model is not modeled currently due to the MELCOR capability to model a single coolant only.
5	Sodium-Concrete Interaction	As a part of the pool chemistry, only eight major chemical reactions are considered in the sodium-concrete interaction model. In terms of sodium-concrete interactions, the SLAM model from CONTAIN will be implemented. The constituents considered include those species from the sodium-concrete interaction, and those with sodium with water content in the concrete.
6	Debris Bed/Concrete Cavity Interaction	This model is not considered.

In the following section of Chapter 2, the CONTAIN-LMR model is described, followed by a discussion of the CONTAIN-LMR coding of the model. Finally, the implementation approach to migrate the CONTAIN-LMR model into MELCOR is given in Chapter 3.

2.1. Review of CONTAIN-LMR Models

A number of sodium chemistry reaction models are being added to MELCOR based on models found in CONTAIN-LMR [Murata 1993]. The chemistry models include: atmosphere chemistry, sodium spray, and a sodium pool model. These three chemistry models are summarized in this section. For complete details of the chemistry models, refer to the CONTAIN-LMR manual [Murata 1993]. Additionally, this section describes the models of the two-condensable option and

the sodium-concrete interaction from CONTAIN-LMR. The debris interaction model from CONTAIN-LMR will not be implemented in MELCOR because the underlying conceptual model does not apply for the metallic fuel type preferred in domestic SFR design. Though code architecture differs significantly between MELCOR and CONTAIN-LMR, these models will be coded similarly and code-to-code validation will be performed to assure that the model transfer was performed correctly.

2.1.1. Sodium Spray Fire

Of the two basic types of sodium fires postulated in sodium-cooled fast reactors, spray- and pool-sodium fires, spray fires are generally considered to be more energetic. The large surface area of the droplet in spray versus the pool surface area causes sodium sprays to burn at a higher rate than a sodium pool containing the identical amount of sodium. Pipe breaks are typically modeled as sodium-spray fire. The sodium is assumed to be released through the break by ejecting upward and impacting on the ceiling of the room where a sodium liquid is formed and then breaks up to form droplets [Tsai 1980]. These droplets are modeled as a sodium spray. The interaction of the sodium spray with oxygen and available moisture in the atmosphere of the room creates the sodium-spray fire phenomena.

The model for the sodium-spray fire is based on the phenomenological model used in NACOM, a code developed and tested at Brookhaven National Laboratory [Tsai 1980]. However, CONTAIN-LMR did not include the sodium reaction with water vapor as in NACOM. The trajectory of the droplets is assumed to be a downward flow with a terminal velocity. The combustion rate of the spray fire is integrated over the droplet's fall to obtain the total sodium burned mass, as functions of droplet size, fall velocity, and atmospheric conditions.

The user specifies the mean droplet diameter for the sodium spray, then an initial size distribution is determined using the Nukiyama-Tanasama correlation [Tsai 1980]. The current default mean droplet diameter is set at 0.001 m. This model also requires a user input fall height 'HITE'. In addition, this model requires the user to specify the mole fraction of Na_2O_2 produced by the spray fire. This mole fraction is currently set at 1.0 as default. Two main reactions with oxygen are modeled as shown in Reactions (2-7) and (2-8) in Section 2.1.3.

The combustion energy is computed based on the mole fraction of sodium ($\mathbf{F_{peroxide}}$) to peroxide (Na_2O_2) as given by the following correlation:

$$\mathbf{S} = \frac{\mathbf{1.3478 \cdot F_{peroxide}}}{\mathbf{1.6957 - 0.3479 \cdot F_{peroxide}}} \tag{2-1}$$

Heat combustion, E_{spray} (J) is then calculated as

$$\mathbf{E_{spray}} = \mathbf{(1 - S) \cdot 9.1797 \times 10^6 + S \cdot 10.46 \times 10^6} \tag{2-2}$$

The duration of this source and the available oxygen determines the combustion time and the amount of the by-products and heat content to be generated. In the absence of better information regarding the kinetics of the oxidation process, the value of 1 for the ratio of peroxide over the sum of the peroxide and monoxide is often used. Tests have shown that the peroxide indeed dominate the reaction products, particularly when combusting in air.

2.1.1.1. CONTAIN Coding

The SPRAY routine documents the sodium spray fire model. The input routine for this model is through ISPRAY.

In the SPRAY routine, the following information is used:

- Droplets are assumed at 1.015×10^5 Pa and saturation temperature.
- Mass fraction of Na_2O_2 is estimated based on the user-specified input.
- Heat is estimated based on the above mass fraction.
- Selection of drop size distribution is based on the user-specified mean droplet diameter.
- Determination of the spray source is based on the user-specified data.
- Integration of the droplet fall and reactions is estimated.

The SPRAY routine only calls VELT routine for estimating the terminal velocity and Reynolds number. The SPRAY routine also calls SORSPR routine for the spray source. The current VELT routine only treats downward falling droplets.

Only SPRAY and VELT subroutines will be implemented into MELCOR, with proper interface variables for communicating with other packages in MELCOR.

2.1.2. Sodium Pool Fire

This sodium pool fire model is taken from the SOFIRE II code developed from the results of pool fire tests [Beiriger 1973]. SOFIRE II model was based on the verification of experiments, which included a large test vessel in a series of thermodynamic parameter tests to study the effect of oxygen concentration on the system pressure, sodium burning rates, and heat transfer rates. This vessel has a diameter of 3.05 m (10 ft), with a height of 9.14 m (30 ft) and contains 62.3 m^3 (2200 ft^3) of gas at the standard condition. In the lower section of the vessel, a 0.5574 m^2 (6 ft^2) steel pan was installed on a spider off of the floor of the vessel. The pan was insulated with fire brick and mounted below a feed line from an external sodium preheat tank. Thermocouples were mounted in or on the sodium pool volume, steel pan, pan insulation, gas volume, and vessel walls. This experiment is referred to as a one-cell experiment. A two-cell experiment was also used to validate this model [Beiriger 1973].

The main pool fire reaction for this model is given as:

$$(\mathbf{1}+\mathbf{f_1})\cdot\mathbf{2}\cdot\mathbf{Na}+\ \mathbf{O_2}\rightarrow\mathbf{2}\cdot\mathbf{f_1}\cdot\mathbf{Na_2O}+(\mathbf{1}-\mathbf{f_1})\cdot\mathbf{Na_2O_2}+\mathbf{q(reaction)} \qquad (2\text{-}3)$$

where f_1= fraction of total oxygen consumed that reacts to form monoxide and q(reaction) is 9.04540×10^6 J/kg and 1.09746×0^7 J/kg for the monoxide and peroxide, respectively [Murata 1993].

The above reaction requires oxygen in the air to diffuse to the sodium pool. CONTAIN-LMR uses a diffusion constant, D_O (m^2/s) for oxygen-nitrogen mixtures different than that of SOFIRE II [Murata 1993]:

$$D_0 = 6.4315\times10^{-5}\frac{T_{film}^{1.823}}{P} \quad (2\text{-}4)$$

where T_{film} = average temperature of the pool and atmosphere (K) and P = system pressure (Pa).

The user must specify the amount of the products and reaction energy to the pool and to the atmosphere layer of the cell through fractional inputs. The fractional inputs include:

- f_2 is the fraction of sensible heat from the reaction to the pool. The remainder will be directed to the atmosphere layer of the cell.
- f_3 is the fraction of Na_2O product that enters the pool as a solid after the fire. The remainder will be directed to the atmosphere as aerosols.
- f_4 is the fraction of Na_2O_2 product that enters the pool as a solid after the fire. The remainder will be allocated to the atmosphere as aerosols.

Note that the sodium burning rates calculated by this model depend on the temperature differences between the pool and the atmosphere. This difference is assumed to set up turbulent natural convection above the pool surface—the greater the differential, the greater the burning rate would be. Thus radiative heat transfer between the pool and its surroundings may result in different burning rates.

Note that the description below is provided to document what is in CONTAIN-LMR. It may not be used when the pool fire model is implemented into MELCOR, since MELCOR has its own pool boiling heat transfer.

2.1.2.1. CONTAIN Coding

This sodium pool fire model is associated with the sodium pool in the reactor cavity area. The lower cell input must be invoked in order to use this model. This modeling is to include any heat transfer equations that are specifically designed for sodium forming a lower cell pool. In CONTAIN-LMR, thermal radiation exchange between the burning sodium pool and heat structures are being modeled. This model is called within the lower-cell physics routine. In RHCNTR subroutine, where the lower cell controls are done, it calls lower cell layers to set up the physics such as the intermediate and concrete layers. Then, it calls the pool layer, which calls the PFIRE routine to perform sodium pool fire calculations using Eq. (2-3) and the fractional inputs above. The calculations include mass and energy estimate of the reaction, including the estimate of the reactants, sodium from the pool and the oxygen from the atmosphere, via Eq. (2-4) for the diffusion rate, and the products, sodium monoxide and sodium peroxide. The allocation of the product masses to the pool and atmosphere are functions of the user-defined values or by default.

The PFIRE subroutine will be implemented into MELCOR with proper interface variables to communicate with other packages in MELCOR. In CONTAIN-LMR, pool thermal radiation exchange between heat structures is modeled.

2.1.3. Atmospheric Chemistry

Depending on the accident scenarios, the sodium coolant may occur as vapors that could react chemically with any oxygen or water present. These reactions are exothermic, which can add

thermal load to the containment system. In addition, any hydrogen generated by the sodium chemical reactions may have additional consequences, such as hydrogen explosions. A number of sodium chemistry reactions are considered.

2.1.3.1. Gas Chemistry

The first reaction considered is:

$$\mathbf{Na + H_2O\ (l)\ \rightarrow NaOH + \frac{1}{2}H_2} \qquad (2\text{-}5)$$

Reaction (2-5) is assumed to occur only for liquid phase water and sodium in contact on an aerosol particle, mingling aerosol deposits and condensate films on surfaces. Because the water is required to be liquid, the experimentally observed inhibiting effect of oxygen on reactions of water vapor and sodium is assumed to be inapplicable. This requirement assumes that either the temperature is relatively low (below the critical point of water) and the presence of traceable amount of liquid water. As shown in this reaction, hydroxide is expected to be the principal reaction product with water at low temperatures or with excess water. Conversion from hydroxide to monoxide is not modeled.

For this reaction, Na species include Na (g) and NaOH. Other materials involve H_2O(l) and H_2.

The second reaction is:

$$\mathbf{2\ Na + H_2O\ (g)\ \rightarrow Na_2O + H_2} \qquad (2\text{-}6)$$

This reaction is used when the phase of water is not liquid. It is presumably correct at high temperatures with excess sodium. At low temperatures with excess sodium, the use of reaction (2-14) may produce excess hydrogen per mole of water. This reaction is also appropriate when water vapor is present, particularly when there is an excess of water vapor over oxygen. In this case, the water vapor is assumed to react not only with sodium vapor in the atmosphere, but also with sodium in aerosol form or in the form of aerosol deposits or films on surfaces. However, the reaction rate for reaction (2-14) at the surface with water is assumed to be limited by the evaporation rate of water from the surface. The sodium species include Na and Na_2O. Other species include H_2O (g) and H_2.

After the reactions with water, if any, oxygen in the atmosphere is assumed to react with sodium to form the monoxide and peroxide, respectively as follow:

$$\mathbf{2\ Na + \frac{1}{2}O_2\ \rightarrow Na_2O} \qquad (2\text{-}7)$$

$$\mathbf{2\ Na + O_2\ \rightarrow Na_2O_2} \qquad (2\text{-}8)$$

For reaction (2-7) and (2-8) for monoxide versus peroxide as products, this fraction relies on the input fraction parameter "FRNA2O" which represents the fraction of monoxide in the total reactions with oxygen. Reactions (2-5) to (2-8) also are assumed to occur with sodium aerosols, sodium aerosol deposits, and sodium films in that order.

Two subsequent reactions take place when peroxide and monoxide have been formed. The first subsequent reaction is for peroxide reacting with sodium:

$$\mathbf{Na_2O_2 + 2\,Na \rightarrow 2\,Na_2O} \quad (2\text{-}9)$$

This reaction is always assumed to occur if the peroxide and condensed sodium are in contact as a consequence of being present on the same aerosol particle or as a consequence of the mingling of the aerosol deposits and condensate film on a surface. The order is aerosol particles then aerosol deposits.

Sodium monoxide and peroxide can react with water to form sodium hydroxide:

$$\mathbf{Na_2O + H_2O\,(g) \rightarrow 2\,NaOH} \quad (2\text{-}10)$$

$$\mathbf{Na_2O_2 + H_2O\,(g) \rightarrow 2\,NaOH + \frac{1}{2}O_2} \quad (2\text{-}11)$$

Water vapor is assumed to react with aerosol particles and aerosol deposits in that order. Again, the user should note that while the hydroxide is expected to be the principal reaction product with water at low temperatures or with excess water, the possible subsequent conversion of the hydroxide to the monoxide is not modeled if conditions change. The chemical reaction models presented here assume that all reaction heat is retained only by the gases present or by the structures; the models ignore the increase in the heat content of the aerosols or aerosol deposits due to an increase in temperature above the temperature of the formation. The heat generated by the surface reactions is assumed to be deposited at surface nodes of the structures involved. This treatment is regarded as conservative.

2.1.3.2. Combustion of Sodium Hydrogen Jets

CONTAIN-LMR models the deflagration of hydrogen in the presence of sodium aerosol particles as ignition sources via the standing flame model for hydrogen burn. If the standing flame model is active in the current volume, each flow path into the volume is monitored for temperatures and concentrations of hydrogen and sodium. If the flow entering has a temperature greater than 533.1 K, a hydrogen mole fraction greater than 0.1, and a sodium density greater than 0.006 kg per cubic meter of hydrogen, and there is at least 8% molar oxygen in the atmosphere, a burn is initiated. If sufficient oxygen is present, all of the hydrogen entering with the sodium is consumed.

$$\mathbf{H_2(g) + 0.5O_2(g) \rightarrow H_2O(g)} \quad (2\text{-}12)$$

where the reaction energy is 1.43×10^8 J/kg of hydrogen consumed. Note that this model requires the donor cell (or volume) information on flow, and state of the gases and aerosols coming into the present cell or volume. Thus this model is considered to be an inter-cell or inter-volume model, rather than an intra-cell or intra-volume model.

2.1.3.3. CONTAIN-LMR Coding

The modeling of the atmospheric chemistry model is complicated, because it involves gases, surfaces, and aerosol reactions. Table 2-2 shows the subroutines in the CONTAIN-LMR code for this model. Based on the above, all of these subroutines will be implemented to MELCOR, with proper interface variables to be communicated with other packages in MELCOR.

Table 2-2. CONTAIN Subroutines for the Sodium Atmospheric Chemistry Fire Model [Murata 1993]

Subroutine	Description
CHEMRX	Controlling routine that calls other subroutines as shown below
CHMGAS	Reactions with gases
CHMREP	Reactions within aerosol particles or within aerosol deposit or condensable film
CHMDEP	Reactions of deposits or film with gases

2.1.4. Sodium-Concrete Interaction

When sodium leaks onto a concrete floor, there is a potential chemical reaction between the sodium and the concrete material. Although the concrete is normally lined with steel to protect against the direct contact of the sodium, there are heat transfers between the liquid sodium and the liners that could potentially heat up the concrete floor, which will cause the concrete to dry out. Both carbon dioxide and moisture released from the concrete can interact with sodium if the liner is penetrated. Thus, a sodium-concrete interaction can occur. The model treatment in CONTAIN-LMR is based on the experiments done at SNL regarding the sodium limestone ablation model (SLAM) [Suo-Anttila 1983, Westrich 1983]. This report provides only a brief description of SLAM and the reader is encouraged to read the previously referenced reports for a more detailed description.

SLAM uses a nodalized representation of the concrete with models for heat transfer, water migration, water and CO_2 evolution, and chemical ablation of exposed concrete surface (see Figure 2-1). As shown in Figure 2-1, SLAM consists of three regions. The uppermost region is the pool region, but the nodalization is associated with the boundary layer where the ablation occurs. Below this region is the dry concrete region. Also shown in this figure, a number of constituents can be included within SLAM, which includes SiO_2, H_2O, Na, H_2, NaOH, Na_2SiO_3, Na_2CO_3, Na_2O, CaO, $CaCO_3$, CO_2, graphite, $MgCO_3$, MgO, inerts, steel, and UO_2. The major reactions considered in SLAM are given later. In SLAM, the boundary layer consists of 12 nodes, while the dry region consists of 15 nodes or more. Each node has the same thickness or size, which varies with the changing dimensions of the dry concrete region. A variable, "del1", is the thickness of the boundary layer and dry concrete regions. This variable is subjected to change in terms of increasing or decreasing in the course of a problem. The initial del1 is 0.003 m. The dry concrete region will increase when the thermal penetration rate of the concrete exceeds the ablation rate and will decrease when the converse is true. The bottom-most region is the wet concrete region where evaporable water may still be found in the concrete as shown in this figure. The number of nodes depends on the number of dry nodes which is given by 50 – ndry + 2.

With these three regions, SLAM computes each region as time passes and penetration occurs, during which each region will change its size and position. The coordinate system of SLAM uses the moving Eulerian system (see more details in [Suo-Anttila 1983]). Below is a brief description of each region.

Pool Region: The pool region contains a sodium pool region with all of the reaction products from the sodium-concrete interaction. Materials are assumed to be well mixed and virtually isothermal.

The pool changes in composition which results in swelling with time during penetration. The swelling is caused by the addition of gases and reaction products of lower density than the reactants.

Dry Region: The dry region contains the dehydrated concrete region and the boundary layer of the pool region. Almost all of the important reactions occur within the boundary layer of the dry region. At the interface, the ablation is presumed to occur by two mechanisms: dissolution and ablation. This region can swell or shrink (it moves with the penetration front).

Wet Region: The wet region is the concrete region that contains water. The distribution of the water is important because it determines the amount which can be evaporated and available for the reactions with sodium at the boundary layer.

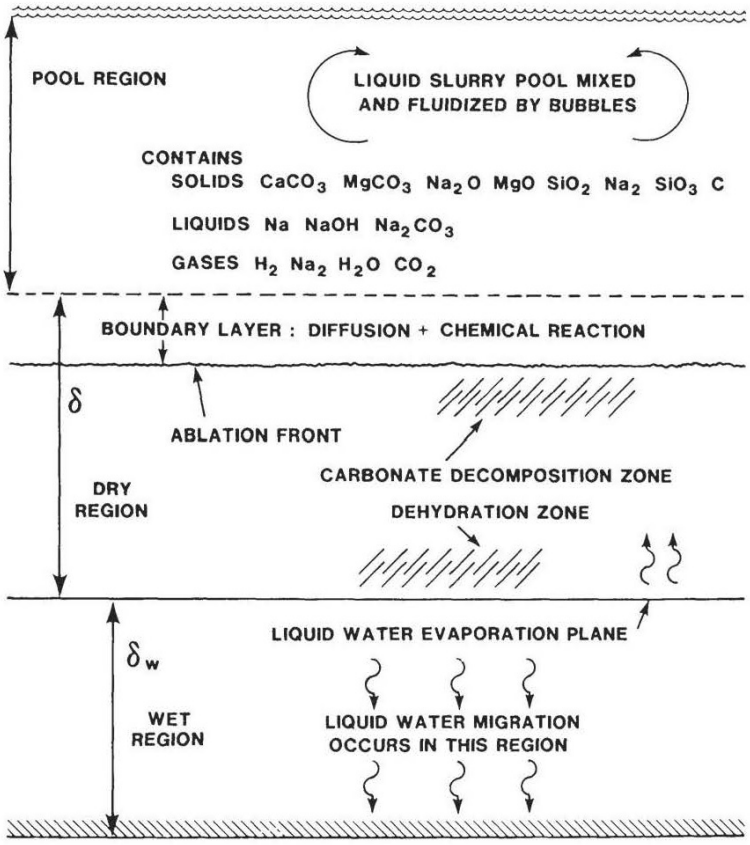


Figure 2-1. Schematic Diagram of SLAM [Suo-Anttila 1983]

Major reactions considered in SLAM are [Suo-Anttila 1983]:

$$\mathbf{H_2O + Na \rightarrow NaOH + 1/2\ H_2} \tag{2-13}$$

$$\mathbf{CO_2 + 2\ Na \rightarrow 4\ Na_2O\ + C} \tag{2-14}$$

$$3\,CaCO_3 + 4\,Na \rightarrow 2\,Na_2CO_3 + 3\,CaO + C \quad (2\text{-}15)$$

$$3\,MgCO_3 + 4\,Na \rightarrow 2\,Na_2CO_3 + 3\,MgO + C \quad (2\text{-}16)$$

$$2\,NaOH + CaCO_3 \rightarrow CaO + H_2O + Na_2CO_3 \quad (2\text{-}17)$$

$$2\,NaOH + SiO_2 \rightarrow Na_2SiO_2 + H_2O \quad (2\text{-}18)$$

Note that SLAM is designed for limestone concrete, which has ignored the possible reaction forming Na_4SiO_4, because of the small quantity of silicates present in the limestone concrete. The reaction with silicates would provide a significant heat source in comparison to the carbonates.

The coordinate system used in SLAM is represented in Figure 2-2. As shown in this figure, SLAM uses a 1-D nodalization to compute all three regions. The moving boundaries at the interfaces of the three regions are shown. For details, refer to [Suo-Anttila 1983].

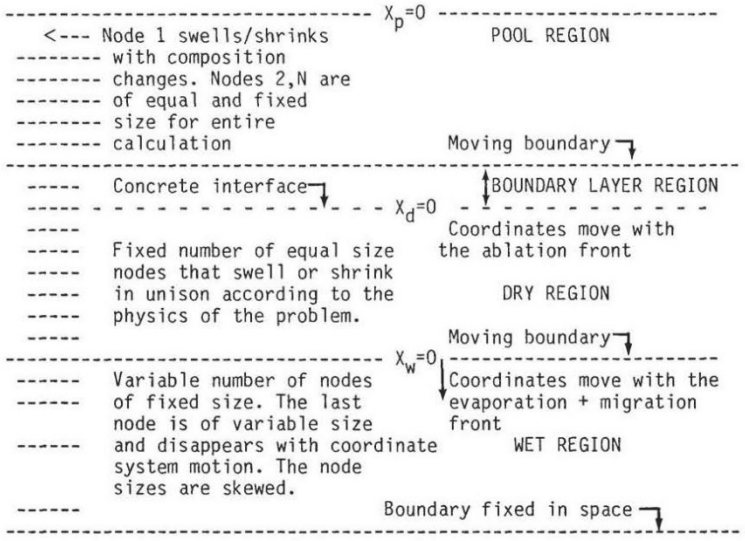


Figure 2-2. The SLAM Systems (subscripts p, d, and w refer to pool, dry, and wet respectively) [Suo-Anttila 1983]

The SLAM model is described in this section. Notably, the SLAM model in CONTAIN-LMR [Murata 1993] works in conjunction with the core debris in the cavity. Thus the SLAM in CONTAIN-LMR may be used with CORCON. However, we would only assume that a sodium pool is present to react with the concrete below.

In the CONTAIN-LMR manual [Murata 1993], the SLAM model had not been validated. The concrete ablation using CORCON and allowing concrete outgassing was under development at that time. Below are the assumptions and restrictions described [Murata 1993]:

- An option to disable concrete ablation and allow only concrete outgassing
- The outgassing option assumes that the concrete is covered with an impenetrable barrier, representing the liner shell.
- The gases removed from the concrete through the SLAM outgassing option are not placed into the atmosphere of a cell, but simply disappear from the problem.

2.1.4.1. CONTAIN Coding

The SLAM model in CONTAIN-LMR is primarily contained in several subroutines, including the interfaces with the CORCON models. The SLAM model uses several calling routines before calling the main SLAM subroutine. The calling sequences allow the understanding of how the SLAM model works. Once called, the SLINPT subroutine is called to initialize the boundary layer, SLAM chemistry data, and concrete information. Within SLINPT, the routine calls SLCHEM for reading chemical reaction data, then CONCPT for determining the concrete array pointers, then SLCOOR for initializing SLAM coordinate system.

To aid the development of SLAM models in MELCOR, the SLAM model output from CONTAIN-LMR includes:

- Average dry region temperature
- Wet-dry interface temperature
- Concrete reaction heat
- Concrete surface heat flux
- Heat flux into the wet zone
- Penetration depth
- Ablation velocity
- Dry zone depth
- Dry zone growth rate
- Dry zone heat sources
- Wet-dry interface heat flux
- Wet-dry interface water partial pressure
- Interface water evaporative flux
- Flux of bound water from the dry zone
- Integral of evaporative and bound water flux
- Flux of bound CO_2 from the dry region
- Integral of CO_2 flux

2.2. Summaries and Conclusions

This chapter summarizes the sodium chemistry models being implemented into MELCOR. A number of subroutines from CONTAIN-LMR for these models can be easily implemented into MELCOR with the appropriate interfaces. The spray model currently can only model the downward spray droplets. Upward spray may require additional modeling change. For the pool fire model, CONTAIN-LMR contains a heat exchange between the sodium fire model and its

surroundings, namely heat structures. Unlike water, a sodium pool fire can reach to 1000 K or higher. The sodium-concrete interaction model may require additional reviews because the CAV package may be involved. This determination will be made in the near future.

3. SODIUM CHEMISTRY (NAC) PACKAGE DEVELOPMENT

A new package "Sodium Chemistry" (NAC) package has been added to MELCOR. In order to activate this package, "NFLUID" must be either 7 for the FSD database or 20 for the SIMMER database for the sodium coolant. This package includes a number of subroutines from CONTAIN-LMR, which include SPRAY, CHEMRX, CHMAER, CHMGAS, CHMREP, CHMDEP and PFIRE. All these subroutines contain interfaces with CVH and RN package variables for transferring chemistry related processes (both heat and mass), including sodium, oxygen, water and the creation of the by-products of sodium burn resulting from the reactions. As shown in

Figure 1-1, a total of five aerosol species are identified, including the reactants and the sodium by-products. Note that the number of default classes in the RN package is shown in Table 3-1. The five RN classes to be tracked within the NAC package include H_2O, Na, NaOH, Na_2O, and Na_2O_2 aerosols. Note that there should be more than five aerosols if including the by-products from the SLAM model (see Section 2.1.4). For now, only five aerosol mappings from NAC are included for the chemistry models, except for the SLAM model. For the SLAM model, the additional aerosols (see the list of solids in Figure 2-1) will be included.

Since the sodium chemistry models in CONTAIN-LMR are usually in the form of correlations, it is recommended that some of the coefficients of the correlations be placed in sensitivity coefficients, allowing the user to over-write as necessary to model his or her specified problem.

Since there is a standard numbering of the package sensitivity coefficients in MELCOR, it was decided to use 8100-8499 as the range for sodium specified models. Other numbers have been used or reserved for other package uses.

Table 3-1. RN Class Compositions

Class	Class Name	Chemical Group	Representative	Member Elements
1	XE	Noble Gas	Xe	He, Ne, Ar, Kr, Xe, Rn, H, N
2	CS	Alkali Metals	Cs	Li, Na, K, Rb, Cs, Fr, Cu
3	BA	Alkaline Earths	Ba	Be, Mg, Ca, Sr, Ba, Ra, Es, Fm
4	I2	Halogens	I_2	F, Cl, Br, I, At
5	TE	Chalcogens	Te	O, S, Se, Te, Po
6	RU	Platinoids	Ru	Ru, Rh, Pd, Re, Os, Ir, Pt, Au, Ni
7	MO	Early Transition Elements	Mo	V, Cr, Fe, Co, Mn, Nb, Mo, Tc, Ta, W
8	CE	Tetravalent	Ce	Ti, Zr, Hf, Ce, Th, Pa, Np, Pu, C
9	LA	Trivalents	La	Al, Sc, Y, La, Ac, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Am, Cm, Bk, Cf
10	UO2	Uranium	UO_2	U
11	CD	More Volatile Main Group	Cd	Cd, Hg, Zn, As, Sb, Pb, Tl, Bi
12	AG	Less Volatile Main Group	Ag	Ga, Ge, In, Sn, Ag
13	BO2	Boron	BO_2	B, Si, P

Class	Class Name	Chemical Group	Representative	Member Elements
14[2]	H2O/Na	Water/Sodium	H_2O/Na	H_2O, Na
15	CON	Concrete	CON	- – -
16	CSI	Cesium iodide	CsI	CsI
17	CSM	Cesium Molybdate	CsM[1]	CsM[1]

[1]Cesium Molybdate (Cs2MoO4) is represented in MELCOR as CSM in order to satisfy the three-character naming limitation in MELCOR

[2]Class 14 is for the coolant, which can be water if the water reactor is modeled or be sodium if sodium coolant is modeled.

The input records described in Section 3.1 are the most current input information. However, these records will be updated.

3.1. NAC Input Records

As indicated in Section 1.1, MELCOR expects an input file residing in the same working directory as the MELGEN/MECLOR inputs. This input file must match the names of the specific liquid metal fluid. For SFRs, an input file name of "TPFNA" or "SIMMER" must be provided; otherwise, the sodium chemistry models will not be invoked.

The MELGEN input records for all chemistry models are given within the NAC package inputs. Note that the format of the input description is structured according to the MELCOR users guide. The NAC_INPUT record is required.

NAC_INPUT – Activation Record

Required.

This record activates the NAC package in MELCOR. When the NAC_INPUT record is absent, then by default, the activation switch is set to not active. It is required that additional aerosol classes, such as NaOH, Na_2O, Na_2O_2, must be defined in RN1_CC record in order for these aerosols to be existed in the problem. See Appendix A for an example of the RN input for these aerosol classes. If this package is active and NFLUID is not equal to 7 or 20, a diagnostic message will be output and the code is stopped.

(1) IACTV

Activation switch for the NAC package. Optional field.

(a) 0 or ACTIVE

RN package Active

(b) 1 or NOTACTIVE

RN package Not Active

(type = integer / character*9, default=0 (active), units = none)

Example

```
NAC_INPUT ACTIVE
```

This record specifies the activation of the sodium chemistry models in MELCOR. In order to use the package records, NFLUID =7 or NFLUID = 20 must be set when the liquid metal fluid property is invoked. In addition, all sodium chemistry models are control volume specified models; therefore, it is necessary to specify the specific CVH volumes to contain these models.

The following subsections describe the MELGEN input records that are optional if the desired sodium models are invoked.

3.1.1. RN Class Mapping

Since aerosols would be generated from the sodium chemistry models, it is necessary to map the sodium product aerosols with the classes identified in the RN package. Table 3-1 lists the current identification of the RN classes.

3.1.1.1. MELGEN Input Record

Based on the sodium chemistry models described here, only five aerosols have been identified: Na, H_2O, NaOH, Na_2O_2 and Na_2O. As shown in Table 3-1, Na is included in Class 2 of the RN Package, since Class 2 is a radionuclide class. When sodium is designated as the coolant, Class 2 should not be used to represent sodium, since it would be modeled in Class 14. A new class for water aerosol should be added. No specified class can be assigned to the rest of the sodium compounds since they are products of the reactions. Therefore, it is necessary for the users to declare new classes for these sodium compounds. MELCOR will check during MELGEN execution if new classes are not declared and provide a warning message in the diagnostic file. Thus, no sodium compound aerosols would be generated and tracked. Thus this input represents all classes to be tracked for the entire problem and it is necessary to map all reactants and by-products' aerosol classes for the problem.

As follows is a description of the MELGEN Input Record as it appears in the updated NAC users guide.

NAC_RNCLASS – Aerosol mapping

Optional

This record is required to map classes from the RN package to NAC package. When sodium is the working fluid, the class 14 becomes sodium with all SCs that map for sodium. Thus the user is required to define the water aerosol class as "H2Oa" for modeling any water reactions, since water in sodium reactor analyses is being treated as a trace material. Thus SC7110 may be modified for water in the new RN class. Similarly, the molecular weight may be input. Only five input variables are required.

(1) NaCL1

RN class number for water. No default

(type = integer, default = none, units = dimensionless)

(2) NaCL2

RN class number for sodium. Default=14 (see Table 3-1)

(type = integer, default = 14, units = dimensionless)

(3) NaCL3

RN class number for NaOH. No default.

(type = integer, default = none, units = dimensionless)

(4) NaCL4

RN class number for Na_2O_2. No default

(type = integer, default = none, units = dimensionless)

(5) NaCL5

RN class number for Na_2O. No default

(type = integer, default = none, units = dimensionless)

3.1.2. Sodium Spray Fires

The sodium spray fire model is an atmospheric model, which requires a sodium source to be specified either from a table or control function. Both mass and temperature are required for the source. Thus it is necessary to specify the CVH volume in which the spray fire is located. The size of the spray droplet and the associated fall height are required. The fall height is used to calculate the terminal velocity of the droplet. Note that the current model only models the downward fall of the spray droplets. Multiple CVH volumes with spray fires can be modeled. To be consistent with CONTAIN-LMR and ability for the code-to-code comparison, Table 3-2 lists the plot variables for this model.

3.1.2.1. **MELGEN Input Record**

To invoke this model for sodium spray fire, a number of input variables are required. Each spray fire model requires the user to input the fall height and mean sodium droplet diameter. These parameters are used to calculate the reaction time and reaction area in the spray fire. Note that the default height is set to CVH height, while the default mean sodium droplet diameter is set at 0.001 m. Note the spray package (SPR) should not be activated while the NAC package is invoked.

As follows is a description of the MELGEN Input Record as it appears in the updated NAC Users Guide.

NAC_SPRAY – Sodium Spray Fire Model

Optional

This model allows the modeling of the sodium spray fire in a given control volume if the sodium spray source is given.

(1) NUM

The number of control volumes to include this model

(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC

Table row index.

(type = integer, default = none, units = none)

(2) CVHNAME

The name of the CVH volume.

(type = character, default = none, units = none)

(3) HITE

Fall height of sodium spray. Default is CVH height.

(type = real, default = CVH volume height, units = m)

(4) DME

Mean sodium droplet diameter.

(type = real, default = 0.001, units = m)

(5) FNA2O2

Fraction of sodium peroxide produced by the spray fire.

(type = real, default = 1.0, units = m)

(6) SOU-TYPE

Sodium spray source type: TF or CF. Default is TF. Note that two tables are expected: mass and temperature/enthalpy

(type = character, default = TF, units = none)

(7) MASS-NAME

Name of the TF or CF for the mass source.

(type = character, default = none, units = kg/s)

(8) THERM-NAME

Name of the TF or CF for the temperature of the source.

(type = character, default = none, units = temperature)

Table 3-2. Plot Variables for Sodium Spray Fire Model

Plot Variable	Description
NAC-SPR-NASM	Total mass of sodium introduced into the control volume [kg]
NAC-SPR-NABM	Total mass of sodium burned [kg]
NAC-SPR-O2M	Total mass of oxygen removed [kg]
NAC-SPR-NA2O2	Total mass of aerosol Na_20_2 added [kg]
NAC-SPR-NA20	Total mass of aerosol Na_20 added [kg]
NAC-SPR-MP	Total mass of sodium added to the pool [kg]
NAC-SPR-EA	Total energy released to the atmosphere [J]
NAC-SPR-EP	Total energy added to the pool [J]
NAC-SPR-NASM	Total mass of sodium introduced into the control volume [kg]

3.1.3. Sodium Pool Fires

For the chemical energy generated by the pool fire, the current CONTAIN-LMR model assumes that the user specifies the fraction of the oxygen in the atmosphere to form sodium monoxide. Additional user inputs including the fraction of: the fire energy, sodium peroxide, and sodium monoxide contained in the pool are required. Sodium by-products are treated as aerosols. In CONTAIN-LMR, thermal radiation exchange between the sodium fire pool and its surroundings (i.e., heat structures) is modeled. For typical light water reactor applications, modeling of radiant heat exchange between the pool surface and heat structures is not important and consequently, such modeling was not possible in MELCOR until recent code improvements have made this possible (described further below)..

The plot variables for this model are presented in Table 3-3.

Table 3-3. Plot Variables for Sodium Pool Fire Model

Plot Variable	Description
NAC-PFI-O2MC	Cumulative O_2 consumed [kg]
NAC-PFI-NABMC	Cumulative Na consumed [kg]
NAC-PFI-NA2O2MC	Cumulative Na_2O_2 consumed [kg]
NAC-PFI-NA2OMC	Cumulative Na_2O consumed [kg]
NAC-PFI-EAC	Cumulative energy to atmosphere [J]
NAC-PFI-EPC	Cumulative energy to pool [J]
NAC-PFI-O2MR	Rate of O_2 consumed [kg/s]
NAC-PFI-NABMR	Rate of Na consumed [kg/s]
NAC-PFI-NA2O2MR	Rate of Na_2O_2 consumed [kg/s]
NAC-PFI-NA2OMR	Rate of Na_2O consumed [kg/s]
NAC-PFI-EAR	Rate of energy to atmosphere [J/s]
NAC-PFI-EPR	Rate of energy to pool [J/s]

3.1.3.1. Additional Model Requirement for Sodium Pool Fire Model

This section describes the modeling needs for this sodium pool fire model to be used effectively and can compare to CONTAIN-LMR and sodium pool fire experiments. The first model is the thermal radiation exchange between the sodium fire pool and the surrounding heat structures.

3.1.3.2. MELGEN Input Record

To invoke this model, a number of input variables are required to model sodium pool fires. Note that an additional input variable is included to simulate the termination of the pool fire in an experiment (i.e., closing the lid of the pool). In addition, other non-NAC records may be needed to model the spreading of the sodium flow in the pool as in some sodium fire experiments, and the thermal radiation exchange between the sodium fire pool and its surrounding heat structures.

As follows is a description of the MELGEN Input Record as it appears in the updated users guides in the following subsections.

3.1.3.2.1. NAC Specific Record

NAC_PFIRE – Sodium Pool Fire Model

Optional

This model allows the modeling of the sodium pool fire in a given control volume. A number of fraction inputs can be specified.

(1) NUM

The number of control volumes to include this model

(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC

Table row index.

(type = integer, default = none, units = none)

(2) CVHNAME

The name of the CVH volume.

(type = character, default = none, units = none)

(3) FO2

Fraction of the oxygen consumed that reacts to form monoxide. 1-FO2 is the remaining oxygen fraction for the reaction to form peroxide. Default is 0.5.

(type = real, default = 0.5, units = none)

(4) FHEAT

Fraction of the sensible heat from the reactions to be added to the pool. The balance will go to the atmosphere. Default is 1.0

(type = real, default = 1.0, units = none)

(5) FNA2O

Fraction of the Na_2O remains in the pool. The balance will be applied to the atmosphere as aerosols. Default is 1.

(type = real, default = 1.0, units = none)

(6) FNA2O2

Fraction of the Na_2O_2 remains in the pool. The balance will be applied to the atmosphere as aerosols. Default is 0.

(type = real, default = 0.0, units = none)

(7) TOFF

Time to turn off the model. This is useful for modeling certain experiments. Default is 1×10^{12} seconds.

(type = real, default = 1×10^{12}, units = seconds)

3.1.3.2.2. CVH Specific Record

CV_PDIA – Specify User Pool Diameter

Optional

This optional input allows the specification of the pool diameter as a constant value or a control function input. The use of this record would override the pool area calculated using the control volume attitude table. The use of the control function would allow the modeling of the pool spreading (i.e., in an experiment).

(1) pDiameter

Two options are allowed. When a real number is encountered, it is treated as a constant diameter for the pool. When character string or an integer is encountered, it is treated as a control function name or number to define the pool diameter change as a function of a parameter. This allows to model spreading effect.

(type = real, default = none, units = meter)

3.1.3.2.3. HS Specific Record

HS_RD2 – Structure-to-Pool-Surface Radiation

Optional

(1) NUMPAIR

Number of allowable surface pairs.

(type = integer, default = none, units = none)

Next data are input as a table with number or rows = NUMPAIR:

(2) N

Table entry index.

(type = integer, default = none, units = none)

(3) IHSRD

Heat structure name surface 1 of the surface pair.

(type = character*16, default = none)

(4) LRBND

Option to identify the side of surface IHSRD1.

(a) -1 or LEFT

Left side surface of the given heat structure.

(b) 1 or RIGHT

Right side surface of the given heat structure.

(type = integer / character*5, default = none, units = none)

(5) ICVRD

Control Volume containing pool surface (surface 2)

(type = character*16, default = none)

(6) VIEW

View factor between surface 1 and surface 2.

It must lie in the range of 0.0 to 1.0.

(type = real, default = none, units = none)

(8) ICFRD1

Optional real-valued control function name whose value is the emissivity of HS surface (surface 1).

(type = character*16, default = NO [see below])

(9) ICFRD2

Optional real-valued control function name whose value is the emissivity of the pool surface (surface 2).

(type = character*16, default = NO [see below])

See additional information on this record's usage in HS Users Guide.

Examples

```
HS_RD2    5 ! n   ihsrd       lrbnd   CV      view     icfrd1     icfrd2
              1  'top head'    left  'CV1'    1.0     'EMISS'     'EMISS2'
              2  'Wall'        left  'CV1'    1.0     'EMISS'     'EMISS2'
              3  'BotHead'     left  'CV1'    1.0     'EMISS'     'EMISS2'
              4  'horiz-int'   left  'CV1'    1.0     'EMISS'     'EMISS2'
              5  'vert-int'    left  'CV1'    1.0     'EMISS'     'EMISS2'
```

3.1.4. Atmospheric Chemistry

This model is the most complicated chemistry model, because it involves a number of components in the atmosphere, such as condensate, aerosol, and gases reactions. Both sodium as coolant and water as aerosols can react on heat structures in the atmosphere. In addition, this model contains a hydrogen burn model that is activated when sufficient sodium is presented, and it is dependent on the donor volume's condition. The inputs for this burn model are included in the BUR package; it is not included in the NAC package. Note that the atmospheric chemistry model is considered semi-mechanistic in nature, because the model is not derived from experiments. Note this model has not been fully tested or validated.

3.1.4.1. **MELGEN Input Record**

This section describes the MELGEN input variables for this model. This record requires the specification of each CVH volume for which this model is included. This record only models the sodium chemistry in the atmosphere of the CVH volume. This model also accounts for the sodium chemistry on the surfaces such as heat structures and aerosols, except the floor when the sodium pool is presented.

To invoke this model for atmosphere chemistry and for the combustion of sodium-hydrogen jets, minimal input is required. When this record is included, it expects the number of CVH volumes to contain this model. The required fraction FRNA2O, the fraction of sodium that produces the monoxide versus the peroxide in the atmospheric reactions of sodium with oxygen, is an input variable.

As follows is a description of the MELGEN Input Record as it appears in the updated users guide.

NAC_ATMCHEM – Sodium Atmosphere Chemistry Model

Optional

This model allows the modeling of the atmosphere chemistry in a given control volume if the sodium is present in the atmosphere.

(1) NUM

The number of control volumes to include this model

(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC

Table row index.

(type = integer, default = none, units = none)

(2) CVHNAME

The name of the CVH volume.

(type = character, default = none, units = dimensionless)

(3) FRNA2O

The fraction of sodium that produces Na2O versus Na2O2 with oxygen (Eq. 1-3).

(type = real, default = 0.5, units = dimensionless)

3.1.4.2. BUR Package Input

This section describes the required input for the sodium-induced standing flame hydrogen burn model. This model is only applicable for sodium reactors when NFLUID =7 or 20 and is intended to model inflow of hydrogen and sodium aerosol in which the hydrogen occurs. Note that when the burn package (BUR) is activated, all water products from the hydrogen burn are treated as traceable quantities and are represented as water aerosol, H2OA. This model assumes the hydrogen burn is achieved if one of two criteria is satisfied:

- Donor volume temperature is greater than 1060.9 K
- Donor volume temperature is greater than 533.1 K, and total sodium flown in the volume is greater than 0.006 kg per H2 gas volume of the donor volume.

In addition to above criteria, two other criteria are required in order for the hydrogen burn to occur:

- Oxygen mole fraction in the present volume must be greater than 0.08.
- Hydrogen mole fraction in the gas inflow must be greater than 0.1.

As follows is a description of the MELGEN Input Record as it appears in the updated users guides.

BUR_NAI – Sodium-Induced Hydrogen Burn

Optional

This model allows the modeling of the sodium-induced hydrogen burn from the inflow of both hydrogen and sodium into the present volume. This model is only functional when NFLUID = 7 or 20.

(1) NUM

The number of control volumes to include this model

(type = integer, default = none, units = dimensionless)

The following data are input as a table with length NUM:

(1) NC

Table row index.

(type = integer, default = none, units = none)

(2) CVHNAME

The name of the CVH volume.

(type = character, default = none, units = dimensionless)

3.2. Summary and Conclusions

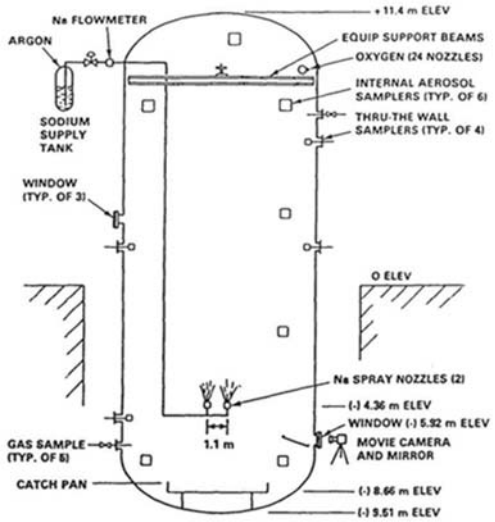
This chapter documents the anticipated MELGEN input records for the NAC package. All input records for the spray fire, pool fire, and atmospheric chemistry models are provided. Only the first two models have been exercised (see Chapter 4 on model testing). We expect to complete atmospheric chemistry model development in the near future (see Chapter 6). The sodium-concrete interaction model inputs are also under development (see Chapter 6).

4. MODEL TESTING

Model development requires testing. Here, we discuss the testing on the implemented models: sodium spray and pool fire models . The testing in this chapter is intended to provide code-to-code comparison with CONTAIN-LMR to identify any issues related to the models' implementation. The models will be validated at a later date when the atmospheric chemistry model has been fully implemented and tested. Currently, only the spray fire and pool fire models are considered complete. We have identified a number of experiments to test the spray fire and the pool fire models. For the spray fire model, the ABCOVE AB5 [Suto 1994] was used. Additional tests, such as Sandia Surtsey T3 [Olivier 2010] tests, will be used. For the pool fire model, the ABCOVE AB1 [Hillard 1979] will be used.

4.1. Sodium Spray Fire Model Testing: ABCOVE AB5 Test

This experiment provided experimental data for validating the aerosol behavior generated by computer codes during a sodium spray fire scenario. This experiment was conducted at the Containment Systems Test Facility at Hanford Engineering Development Laboratory (see Figure 4-1 for the apparatus setup and spray data).



Sodium Spray Data
Na Spray rate (256±15 g/s)
Spray Start Time (13 s)
Spray Stop Time (885 s)
Total Na Sprayed (223±11 kg)
Na Temperature (836.15 K)
Spray Drop Size (1030±50 μm)
Spray size geom. standard deviation (1.4)

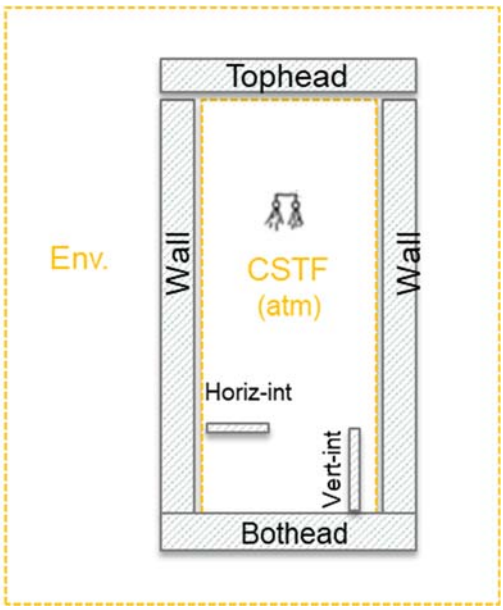
Figure 4-1. Schematics and Spray Data of ABCOVE Sodium Spray Fire Test [Suto 1994]

4.1.1. Experiment Description and Input Models

In this test, the initial sodium spray mass of 223 kg at 836 K was injected into a vessel of 852 m^3 filled with air and O_2 makeup. The validation goals were to observe the sodium combustion during sodium spray, the calculated combustion energy, and aerosol generation. The effect of the pressure and temperature response in the vessel was also of interest. The initial test conditions were 302 K

and 0.122 MPa. The sodium spray characteristics are provided in Figure 4-1. Note that the spray was pointing upward, so the current spray fire model will not correctly capture the sodium residence time since the spray points downward. Nonetheless, for this test a spray fall height was assumed to be 5.15 m from the vessel bottom. This height needs to re-adjust when comparing to the experiment to properly account for the upward flow of the droplets and downward flow of the droplets. To sustain the combustion, a continuous flow of oxygen was provided from 60 to 840 s at a total 47.6 m^3. In terms of the aerosol measurement results, sodium aerosol generated included 60% Na_2O_2 and 40% NaOH. Because the spray fire model currently only models the reactions with oxygen, the formation of NaOH from reacting sodium with water was not accounted for. In addition, the experiment did not fully describe if any reaction occurs in the catch pan if any droplets have not been reacted as shown in Figure 4-2.

The MELCOR input model for this test was based on the model in the MELCOR assessment document [Humphries 2015a]. Although the existing MELCOR model was intended for examining the aerosol behavior, rather than the sodium reactions, it can be modified easily to include the sodium spray model parameters. Figure 4-2 shows the MELCOR model and model description for this test. Similarly, the CONTAIN-LMR input model is derived from this model as well. The MELCOR and CONTAIN-LMR input models developed previously [Humphries 2016a] contained incorrect heat structure surface areas, so that the models have been corrected for this comparison as shown in the following subsection. It is also assumed that if any unreacted droplets fall onto the catch pan or floor the Containment Systems Test Facility (CSTF) volume do not react. Therefore, the pool fire model is not activated.



MELCOR Representation

- Two Control Volumes
  - CSTF volume
  - Environment is a time independent volume to be used for HS boundary condition only
- Six Heat Structures
- No Flow paths
- Na spray rate at 0.256 kg/s from 13 to 885 s at 836.15 K.
- Spray height of 5.15 m is assumed.
- Only reaction to form Na_2O_2 is considered
- O_2 sourced in from 60 s to 840 s at 0.08718 kg/s at 293 K.
- Catch pan is modeled and no pool fire model activated.

Figure 4-2. MELCOR Model for ABCOVE AB5 Test

4.1.2. Code-to-Code Comparison

For this comparison, it is important to identify the differences between MELCOR and CONTAIN-LMR. Below are some of the differences noted:

- CONTAIN-LMR models the cylindrical wall of the CSTF volume in two halves.
- CONTAIN-LMR models water vapor in the atmosphere and currently MELCOR only models water vapor as water aerosol.
- CONTAIN-LMR includes additional inputs:
  - GASWAL thermal radiation models that a simple atmosphere-to-structure radiation model is activated with a small geometric mean beam length used (0.01). It is justified, since the typical mean beam length for a flame is proportional to the flame volume divided by the flame surface area. In the spray fire, the surface area is the sum of all the reacting droplets.
  - In addition, during the spray fire experiment (from observations of the T3 experiment described in the next section), white smoke fills with the entire chamber where the spray fire occurs. This smoke originates from the sodium by-products. These by-products affect a significant amount of the radiation heat transfer from the atmosphere to heat structures.

Based on these differences, the comparison results are shown in Table 4-1. As shown in this table, the spray fire parameters are very similar between MELCOR and CONTAIN-LMR. The other comparisons—the gas pressure, gas temperature and suspended sodium by-product aerosol, namely Na2O2—are presented in Figure 4-3. As shown in this figure, the pressure and temperature values are slightly higher for MELCOR than CONTAIN-LMR. Both codes tend to match parts of the test data as shown in Figure 4-3. In terms of the suspended aerosol, MELCOR underestimates the peak values of the test data, and CONTAIN-LMR overpredicts the results. Note that the experiment yields NaOH which neither MELCOR or CONTAIN-LMR has modeled. In order to validate this test, the atmospheric chemistry model may need to activate. In addition, the upward spray model needs to be included into the spray fire model.

Table 4-1. Comparison of the Spray Fire Results of CONTAIN-LMR and MELCOR for ABCOVE AB5 Test

Parameter	CONTAIN-LMR	MELCOR
Sodium introduced to Control Volume (kg)	2.23232E+02	2.23307E+02
Mass of sodium spray burned (kg)	1.78760E+02	1.77762E+02
Mass of oxygen removed (kg)	1.24355E+02	1.23661E+02
Mass of Na_2O_2 added as aerosol (kg)	3.03169E+02	3.01477E+02
Mass of Na_2O added as aerosol (kg)	0.00000E+00	0.00000E+00
Mass of sodium added to pool (kg)	4.44717E+01	4.55445E+01
Energy released to atmosphere (j)	1.20992E+09	1.14121E+09
Energy added to sodium pool (j)	5.08781E+07	3.71053E+07

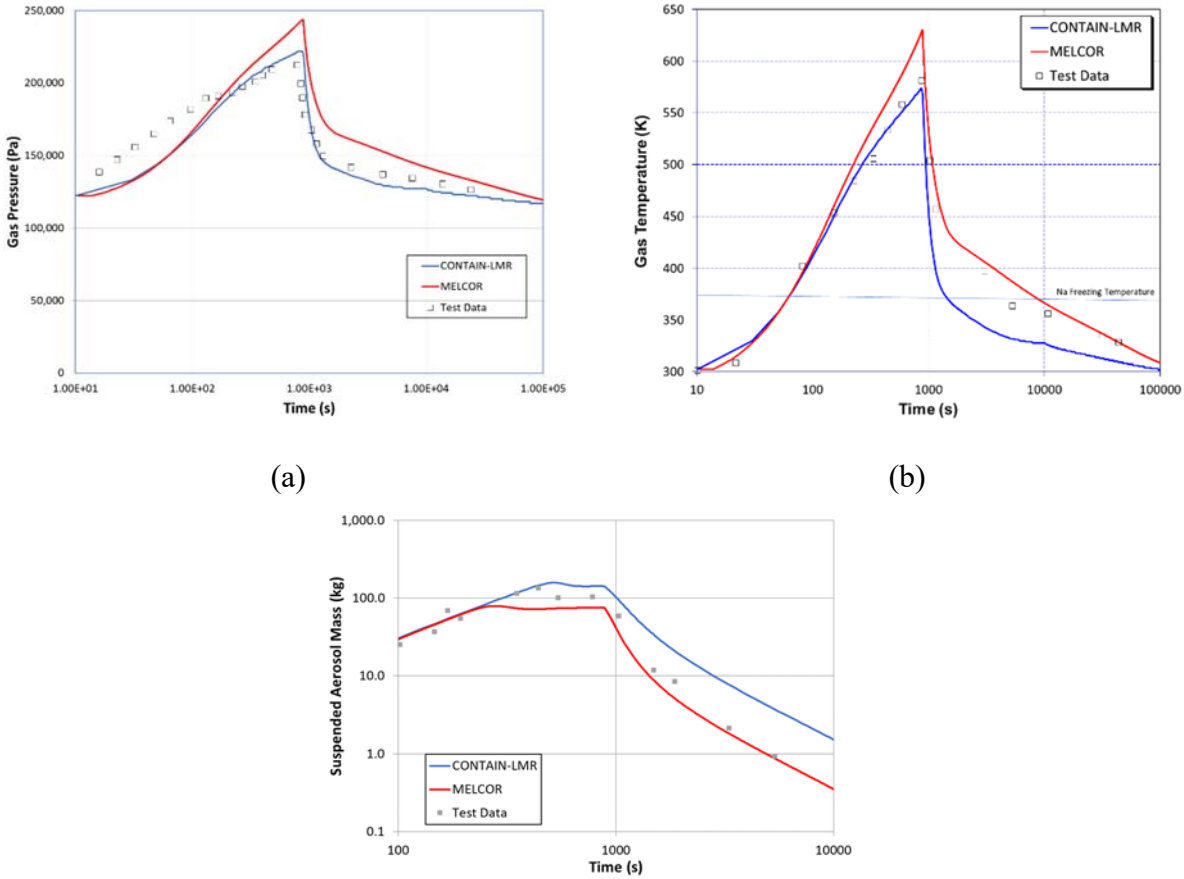


Figure 4-3. Code-to-Code Comparison for ABCOVE AB5 Spray Test

4.2. Sodium Pool Fire Testing: T3 Spray Test

The primary goal of SURTSEY T-3 test was to examine the thermal dynamic behavior of the atmosphere in terms of temperature and pressure. Figure 4-4 shows the schematics of the spray fire tests. As shown in this figure, no instrument was used to measure aerosol generated during the experiment. Only thermocouples and pressure gauges were used. The T3 experimental data and the MELCOR model are shown in Figure 4-5. In this MELCOR model, it assumed a spray droplet size of 2.45 mm and no sodium monoxide was assumed. In addition, any unreacted sodium droplets were allowed to fall onto the floor and accumulate to form a pool, and the pool fire model was activated. In the pool fire model, it is assumed that 0.5 of oxygen reacts to form monoxide, 100% of sensible heat added to the pool, and 100% of Na_2O and 0% of Na_2O_2 enter to the pool. Finally, the pool fire model is terminated at 500 s.

The code-to-code comparison between MELCOR and CONTAIN-LMR for the spray fire is shown in Table 4-1. As shown in this table, most of the parameters are very similar between MELCOR and CONTAIN-LMR, except that the energy added to the pool is smaller for MELCOR. Figure 4-6 compares the gas temperature and pressure of MELCOR and CONTAIN-LMR. As shown in Figure 4-6, both codes match very closely together. However, they are different from the

experimental data. Additional analysis is needed to compare the models against the experimental data, such as the radiation between heat structures and the pool surface or convective heat transfer to the heat structures and material properties. Because of the evidence that a pool fire does occur, the timing for turning off this model may affect the results and comparison to the experiment.

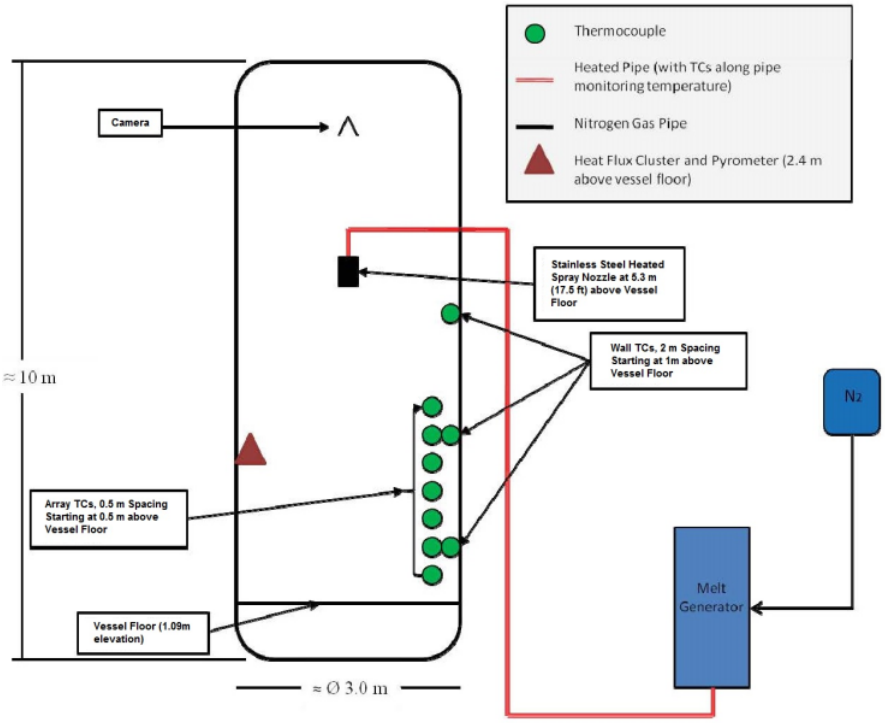
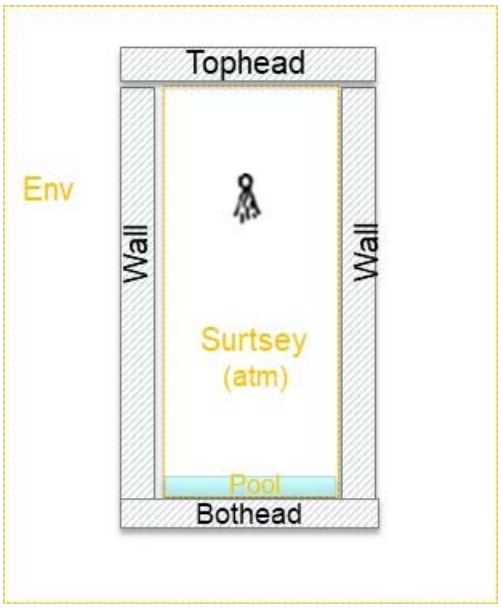


Figure 4-4. SURTSEY Schematics for Sodium Spray Fire Tests [Olivier 2010]

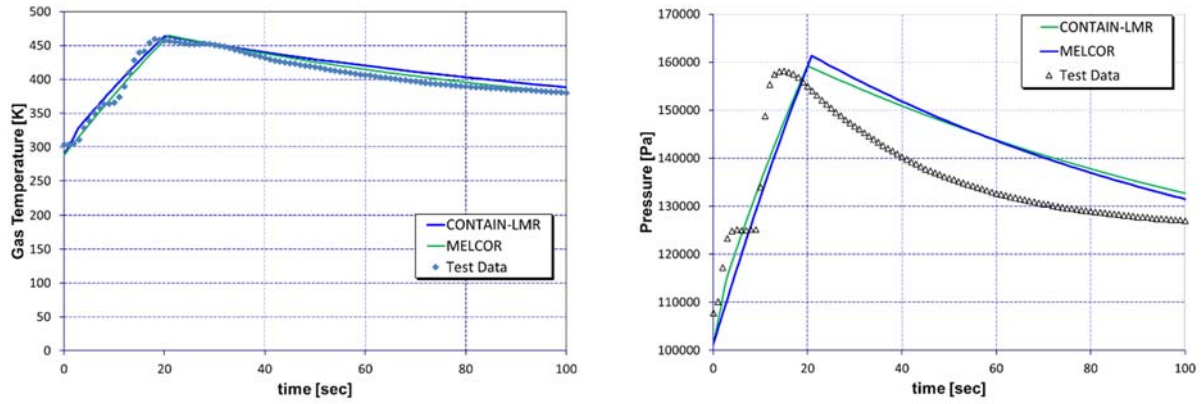


SURTSEY DIMENSION	PARAMETER
Vessel Free Volume	99 m3
Vessel Wall and Heads Thickness	1 cm
Na SPRAY	**PARAMETER**
Na Spray Rate	1 kg/s
Spray Start Time	0 s
Spray Stop Time	20 s
Total Na Sprayed	20 kg
Na Temperature	473.15 K
Spray Drop Size, diameter	3-5 mm
Spray Height	5.3 m
VESSEL CONDITIONS DURING TESTS	**PARAMETER**
Peak Air Temperature (0.33 m from wall)	753.15 K
Peak Overpressure	0.006 MPa
Peak Heat Flux (1.46 m from center)	< 1 kW/m^2

Figure 4-5. SURTSEY T-3 Spray Fire Test Data [Olivier 2010] and MELCOR Model

Table 4-2. Comparison of the Spray Fire Results of CONTAIN-LMR and MELCOR for SURTSEY T3 Test

Parameter	CONTAIN-LMR	MELCOR
Sodium introduced to Control Volume (kg)	2.00000E+01	2.08683E+01
Mass of sodium spray burned (kg)	4.65929E+00	4.71339E+00
Mass of oxygen removed (kg)	3.24124E+00	3.27888E+00
Mass of Na_2O_2 added as aerosol (kg)	7.90194E+00	7.99369E+00
Mass of Na_2O added as aerosol (kg)	0.00000E+00	0.00000E+00
Mass of sodium added to pool (kg)	1.53407E+01	1.61549E+01
Energy released to atmosphere (j)	1.73174E+07	1.72118E+07
Energy added to sodium pool (j)	1.75506E+07	5.58877E+06

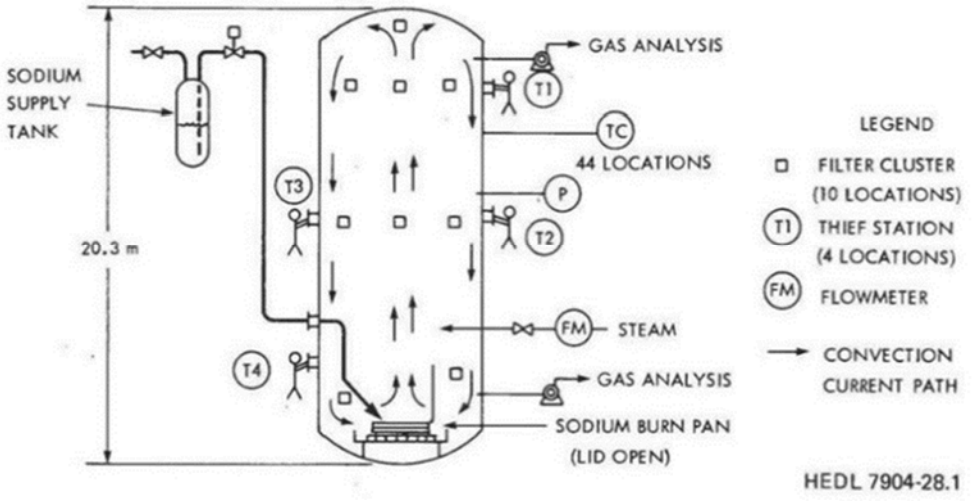


(a) (b)

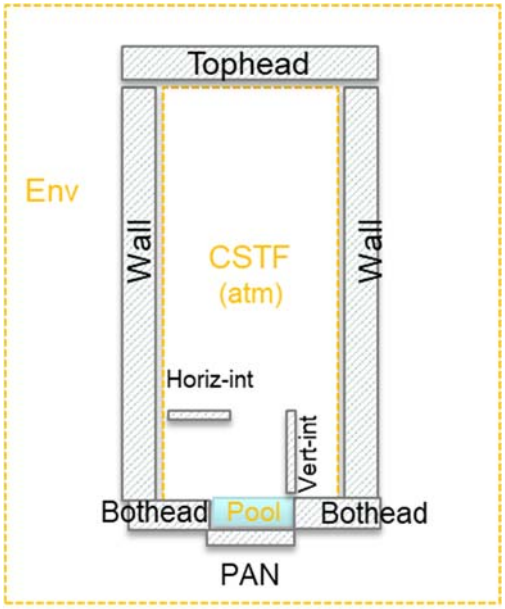
Figure 4-6. Code-to-Code Comparison of Gas Temperature and Pressure for SURTSEY T3 Test

4.3. ABCOVE AB1 Test

This test uses the same CSTF volume as in the ABCOVE AB5 test in Section 4.1 to model the pool fire. Figure 4-7 shows the schematic of the ABCOVE AB1 test. Table 4-3. shows the test conditions for AB1. As shown in this table, the pool fire test contains steam injection. However, there is some moisture in the atmosphere which allows the formation of NaOH. To estimate the NaOH formation, the atmosphere chemistry model must be working. Once this model is implemented completely, more accurate predictions can be provided for this test and for the other tests mentioned in this report.



(a) Experimental Apparatus



MELCOR Representation

- Two Control Volumes
  - o CSTF volume
  - o Environment is a time independent volume to be used for HS boundary condition only
- Six Heat Structures
- No Flow paths
- No O_2 or sodium are sourced into CSTF
- 410 kg of sodium initial pool size
- Lid closes at 1 hour

(b) MELCOR Model

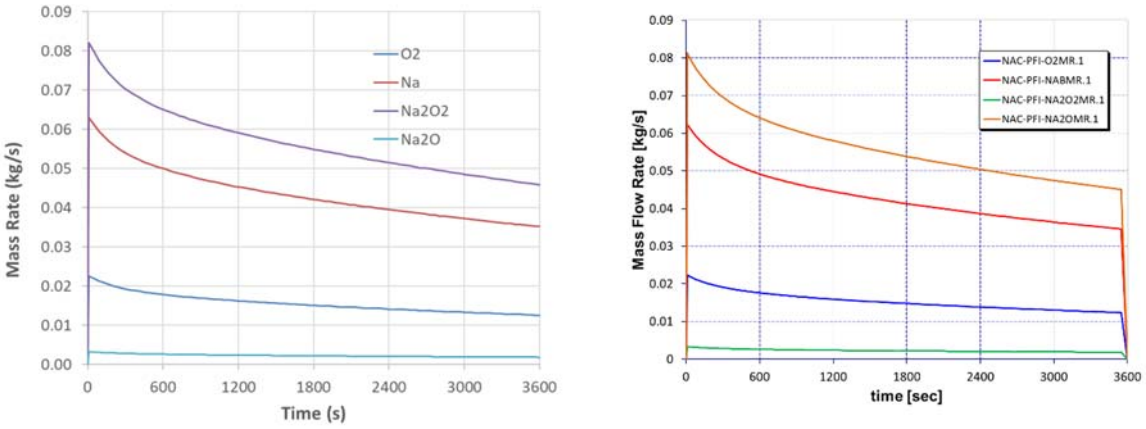
Figure 4-7. Schematic of ABCOVE AB1 Pool Fire Test and MELCOR Model [Hillard 1979]

Table 4-3. Test Conditions for AB1 Test [Hillard 1979]

INITIAL CONTAINMENT ATMOSPHERE	PARAMETER
Oxygen Concentration	19.8%
Temperature (mean)	299.65K
Pressure	0.125MPa
Dew Point	283.15K
Na POOL	**PARAMETER**
Na Source Rate	11.1 g/s
Source Start Time	0 s
Spray Stop Time	3600 s
Total Na Spilled	410 kg
Initial Na Temperature	873.15 K
Burn Pan Surface Area	4.4 m^2
Burn Time	3600 s
Total Sodium Oxidized	157 kg
OXYGEN CONCENTRATION	**PARAMETER**
Initial O_2 Concentration	19.8 vol %
Final O_2 Concentration	14.7 vol %
Oxygen Injection Start	60 s
Oxygen Injection Stop	840 s
Total O_2	47.6 m^3 (STD)
CONTAINMENT CONDITIONS DURING TESTS	**PARAMETER**
Maximum Average Atmosphere Temperature	552.15 K
Maximum Average Steel Vessel Temperature	366.65 K
Maximum Pressure	0.142 MPa
Final Dew Point	233.15 K
Total Aerosol Released as Na	39.9 kg
Fraction of Oxidized Na Released	0.255

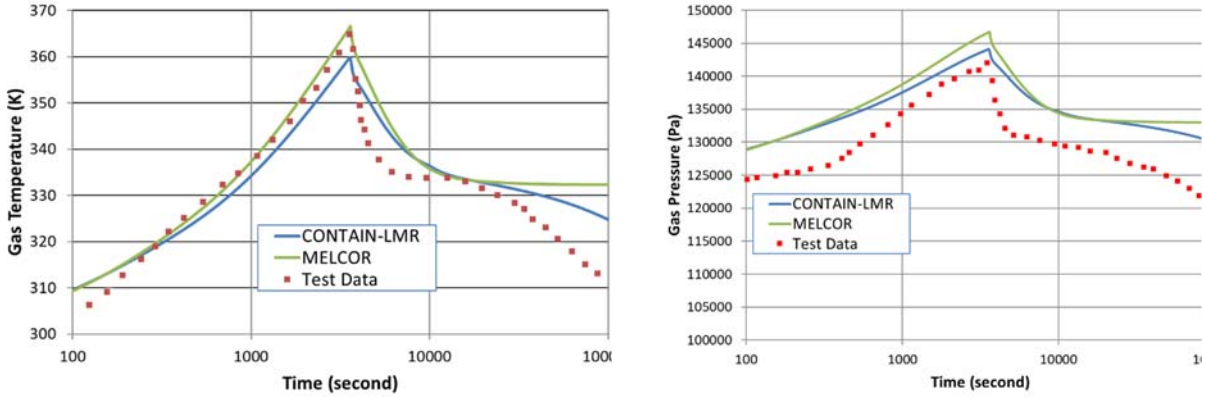
The MELCOR model is provided in Figure 4-7. This model assumes a pool at the bottom of CSTF where the "Bothead" heat structure is located. The initial pool volume is added to the volume altitude table of the CSTF control volume. In addition, because CONTAIN-LMR allows the heat transfer between the pool surface to its surroundings, the MELCOR code was modified since the water pool in a LWR reactor is not important for this heat transfer. Heat structure boundary conditions and stainless steel materials were selected to closely match those in CONTAIN-LMR. A thermal radiation model between pool surface and the heat structures is included via "HS_RD2" record.

The code-to-code comparison of the results from MELCOR and CONTAIN-LMR for the mass flow rates of the pool fire model is shown in Figure 4-8. As shown in this figure, the mass rates compared well between the two codes. For the gas temperature and pressures, Figure 4-9 shows that they match well, except near the end. In terms of comparing to the test data, both overpredict the pressure at the beginning and at the end of the test. Figure 4-10 shows the comparison for the suspended aerosol in the CSTF. As shown in this figure, both MELCOR and CONTAIN-LMR match well with the experimental data.



(a) CONTAIN-LMR (b) MELCOR

Figure 4-8. Code-to-Code Comparison of ABCOVE AB1 Test for Mass Flow Rates



(a) (b)

Figure 4-9. Code-to-Code Comparison of ABCOVE AB1 Test for Temperature and Pressure

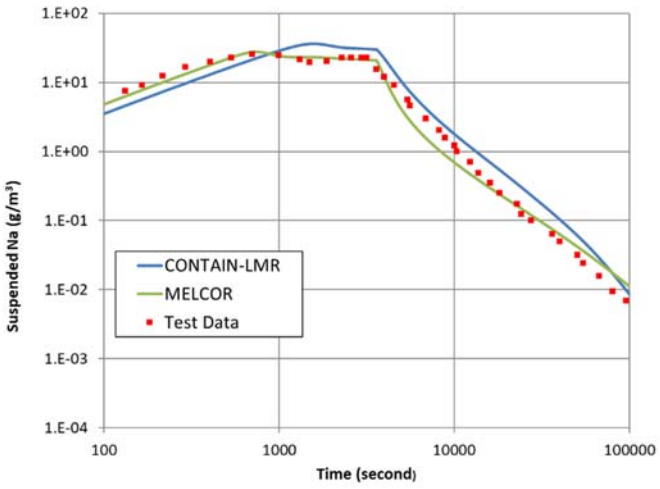


Figure 4-10. Code-to-Code Comparison of ABCOVE AB1 Test for Suspended Aerosol

5. CONCLUSIONS

This report documents the FY17 progress of the NAC package development. The implementation of the spray fire and pool fire models into MELCOR has been completed. The development testing of these two models has been performed and compared against the results of CONTAIN-LMR to ensure that the implementation is done correctly (i.e., code-to-code comparison is complete). The comparison testing used the available spray and pool fire experiments, such as the spray fire experiments (ABCOVE AB5 and T3), and pool fire experiment (ABCOVE AB1). The code-to-code comparison results show that both spray and pool fire models are matched well in terms of the combustion rates and production rates. In terms of comparing to the experimental or test data, both codes compared well at some portions of the data. A version of MELCOR with the sodium spray fire and pool models is expected to be released in first quarter of 2018 calendar year. Note the MELCOR models used may need further refinement to better compare and characterize the experiments. Thus, additional validation testing is required to test these models using refined MELCOR models.

6. EXPECTED TIMELINE FOR THE COMPLETED CODE RELEASE, REMAINING MODELS, AND VALIDATION TESTS

This chapter documents our intention to complete the remaining sodium chemistry models discussed in Chapter 2. In addition, we will need to validate the models with experiments. Experimental model validation will depend on our level of funding. Only two sodium models have been fully implemented into MELCOR; the atmospheric chemistry model (see Sections 2.1.3 and 3.1.4) has largely been implemented into the NAC package. The sodium-concrete interaction model as described in Section 2.1.4 has not yet been implemented into MELCOR; however, the plan and review of the CONTAIN-LMR coding for this model has begun. Table 6-1 below shows the expected schedule to complete these two sodium models and conduct the model validations. Note that there is currently no atmospheric chemistry experiments for the model to be validated against. Thus for this model, only the code-to-code comparison will be provided. Table 6-1. shows the remaining tasks to be completed in 2018 and 2019.

Table 6-1. Expected Completion of the Tasks Remaining to Develop the MELCOR Sodium Chemistry (NAC) Package

Task	Expected Completion Date*
1. Complete the Atmospheric Chemistry Model	1st Quarter of 2018
2.Validation testing of the spray fire, pool fire, and atmospheric chemistry models	2nd Quarter of 2018
3. Complete the Sodium-Concrete Interaction Model (SLAM)	2nd Quarter of 2019**
4. Validate the SLAM model	4th Quarter of 2019**

*Calendar year

**Assuming the same effort as FY18

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APPENDIX A – EXAMPLES OF SODIUM AEROSOL INPUTS

This appendix shows the partial inputs of RN for most of the sodium chemistry modeling when using the NAC package. RN1_CC record is needed to add the sodium, sodium compounds, and water aerosols. The sodium compounds are those sodium materials generated during a sodium chemistry event as listed in Chapter 2 of this report. In addition to RN1_CC records, the user needs to modify the sensitivity coefficients associated with these classes. An example input is shown below.

```
RN1_CC  !num    name   comp number
         1      XE     2
         2      CS     1
         3      BA     2
         4      I2     2
         5      TE     2
         6      RU     2
         7      MO     2
         8      CE     2
         9      LA     2
        10      UO2    2
        11      CD     2
        12      AG     2
        13      BO2    2
        14      H2O    3   ! Na
        15      CON    2
        16      CSI    2
        17      CSM    2
        18      H2OA   3
        19      NAOH   3
        20      NA2O2  3
        21      NA2O   3
!
! all new classes are required to input C7120, C7170
!   7130, 7136, 7141, 7102,  7111, 7120, 7131, 7132, 7170
!   7101, 7110
```

```
RN1_CSC 25 ! N  SCnumber   ClassName   Value       Index1
Index2
! vapor pressure
            1  7110       H2OA        3000.0      1          1
            2  7110       H2OA        18000.0     1          2
            3  7110       H2OA        8.875       1          3
            4  7110       H2OA        0.0         1          4
            5  7110       H2OA        -1.0        2          1
! molecular weight
            6  7120       H2OA        18.016      1
            7  7120       H2OA        18.016      2
! vapor pressure - set to same as UO2, except boiling point
            8  7110       NAOH        1663.0      1          1
            9  7110       NAOH        32110.0     1          2
           10  7110       NAOH        11.873      1          3
           11  7110       NAOH        0.0         1          4
! molecular weight
           12  7120       NAOH        39.99      1
           13  7120       NAOH        39.99      2
! vapor pressure - set to same as UO2
           14  7110       NA2O2       1500.0      1          1
           15  7110       NA2O2       32110.0     1          2
           16  7110       NA2O2       11.873      1          3
           17  7110       NA2O2       0.0         1          4
! molecular weight
           18  7120       NA2O2       78.98      1
           19  7120       NA2O2       78.98      2
! vapor pressure - set to same as UO2
           20  7110       NA2O        1500.0      1          1
           21  7110       NA2O        32110.0     1          2
           22  7110       NA2O        11.873      1          3
           23  7110       NA2O        0.0         1          4
! molecular weight
```

24	7120	NA2O	61.98	1
25	7120	NA2O	61.98	2

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